Overview of TSUNAMI

TSUNAMI

Tools for Sensitivity and UNcertainty Analysis Methodology Implementation

What is TSUNAMI?

- Tools for Sensitivity and UNcertainty Analysis Methodology Implementation
- TSUNAMI utilizes first-order-linear perturbation theory to produce the sensitivities of a computed k_{eff} value to constituent cross-section data.
- The energy-dependent sensitivity data for each reaction of each nuclide in a system model can be quickly computed using TSUNAMI's 1-D and 3-D analysis tools.
- These sensitivity data can be coupled with cross-section-covariance data to produce an uncertainty in k_{eff} due to uncertainties in the evaluated nuclear data.
- Provides an advanced method to assess system similarity based on sensitivity and uncertainty data.

TSUNAMI Development History

- Current ORNL work in sensitivity and uncertainty (S/U) analysis began in 1997
- ORNL had previously performed much S/U work in fast reactor analysis in 1970s – 1980s (FORSS)
  - Eigenvalue and generalized perturbation theory
  - Depletion perturbation theory
  - Shielding
- Foundation for current work presented in NUREG/CR-6655 documents, 1999 (3-year NRC funding)
- Three-dimensional Monte Carlo capability developed in 1999 (3–year EMSP funding)
- Additional research is ongoing (DOE NCSP, DOE EM, NRC)

Perturbation Theory

The relative change in k due to a small perturbation in a macroscopic cross section, Σ, of the transport operator at some point in phase space r can be expressed as

$$S_{k,\Sigma(\vec{r})} \equiv \frac{\Sigma(\vec{r})}{k}\frac{\partial k}{\partial \Sigma(\vec{r})} = -\frac{\Sigma(\vec{r})}{k}\frac{\left\langle \phi^{\dagger}(\vec{\xi})\left(\frac{\partial A\left[\Sigma(\vec{\xi})\right]}{\partial \Sigma(\vec{r})} - \frac{1}{k}\frac{\partial B\left[\Sigma(\vec{\xi})\right]}{\partial \Sigma(\vec{r})}\right)\phi(\vec{\xi})\right\rangle}{\left\langle \phi^{\dagger}(\vec{\xi})\frac{1}{k^2}B\left[\Sigma(\vec{\xi})\right]\phi(\vec{\xi})\right\rangle}$$

where

ϕ = neutron flux;
$\phi^{\dagger}$ = adjoint neutron flux
k = k_{eff}, the largest of the eigenvalues
A = operator that represents all of the transport equation except for the fission term
B = operator that represents the fission term of the transport equation
Σ = problem-dependent resonance self-shield macroscopic cross sections
$\vec{\xi}$ = phase space vector; and
$\langle\ \rangle$ indicate integration over space, direction and energy variables.

TSUNAMI-3D Sequence

- Eigenvalue perturbation theory calculations based on KENO V.a multigroup Monte Carlo transport.
- Problem-dependant resonance self-shielded cross sections and implicit effect computed with 1D continuous energy transport code – CENTRMST.
- Cross section processing, forward and adjoint transport calculations, sensitivity coefficient generation and uncertainty analysis automatically run from a single input.

TSUNAMI-3D Sequence

- Uses 3D Monte Carlo calculations (KENO V.a) to score spherical harmonic moments of forward and adjoint flux:

$$\tilde{\phi}^{\ell}_{g,i} = \frac{\sum_{k=1}^{K} Y^{\ell}(\Omega_{\mathbf{k}})\, w_k\, T_{k,i}}{V_i \sum_{k=1}^{K} w_k}$$

tracklength estimator for ℓ_{th} moment, in group-g, interval-i

- Folds forward and adjoint moments to produce nuclide, energy & cross section dependent sensitivity profiles by spatial zone:

sensitivity coefficient for capture

$$S_{c,g}(z) \cong -\frac{\sigma_{c,g}}{D} \left\langle \Phi(\mathbf{r},E,\Omega)\, \Phi^{*}(\mathbf{r},E,\Omega) \right\rangle$$

$$\rightarrow \frac{-\sigma_{c,g}}{D} \sum_{i \in z} \sum_{\lambda} \tilde{\phi}^{\lambda}_{g,i}\, \tilde{\phi}^{*\lambda}_{g,i}\, V_i$$

Complete Sensitivity Coefficient Includes Effects of Changes in Self-Shielded Cross Sections

- The ***"explicit"*** effect is sensitivity of k_{eff} to changes in multigroup cross sections appearing transport equation

- The ***"implicit"*** effect is sensitivity of k_{eff} to cross section perturbations caused by changes in self-shielding
  - **<u>Example</u>: perturbation in $\sigma^{(H)}$ changes self-shielded $\sigma^{(U238)}$ => cross section data may be sensitive to changes in other data**

$$S_{\alpha_x;\alpha_j} = \frac{\alpha_j}{\alpha_x}\frac{\partial \alpha_x}{\partial \alpha_j}$$

α_x = shielded cross section
α_j = data used in resonance calculation

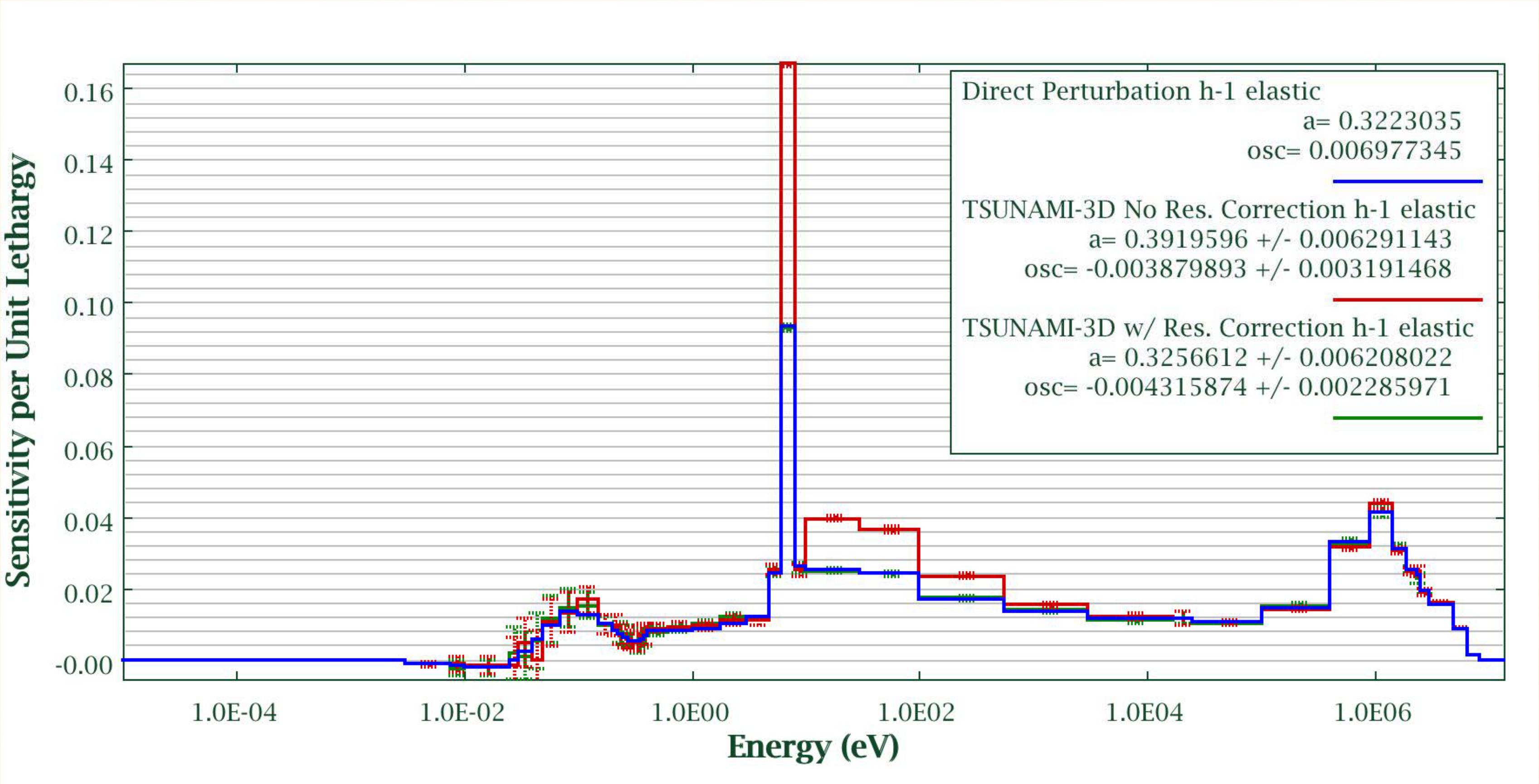
- The implicit effect can be propagated to k_{eff} via the chain rule for derivatives and combined with the explicit to form the complete sensitivity coefficient.

Improved Results by Including Implicit Effect

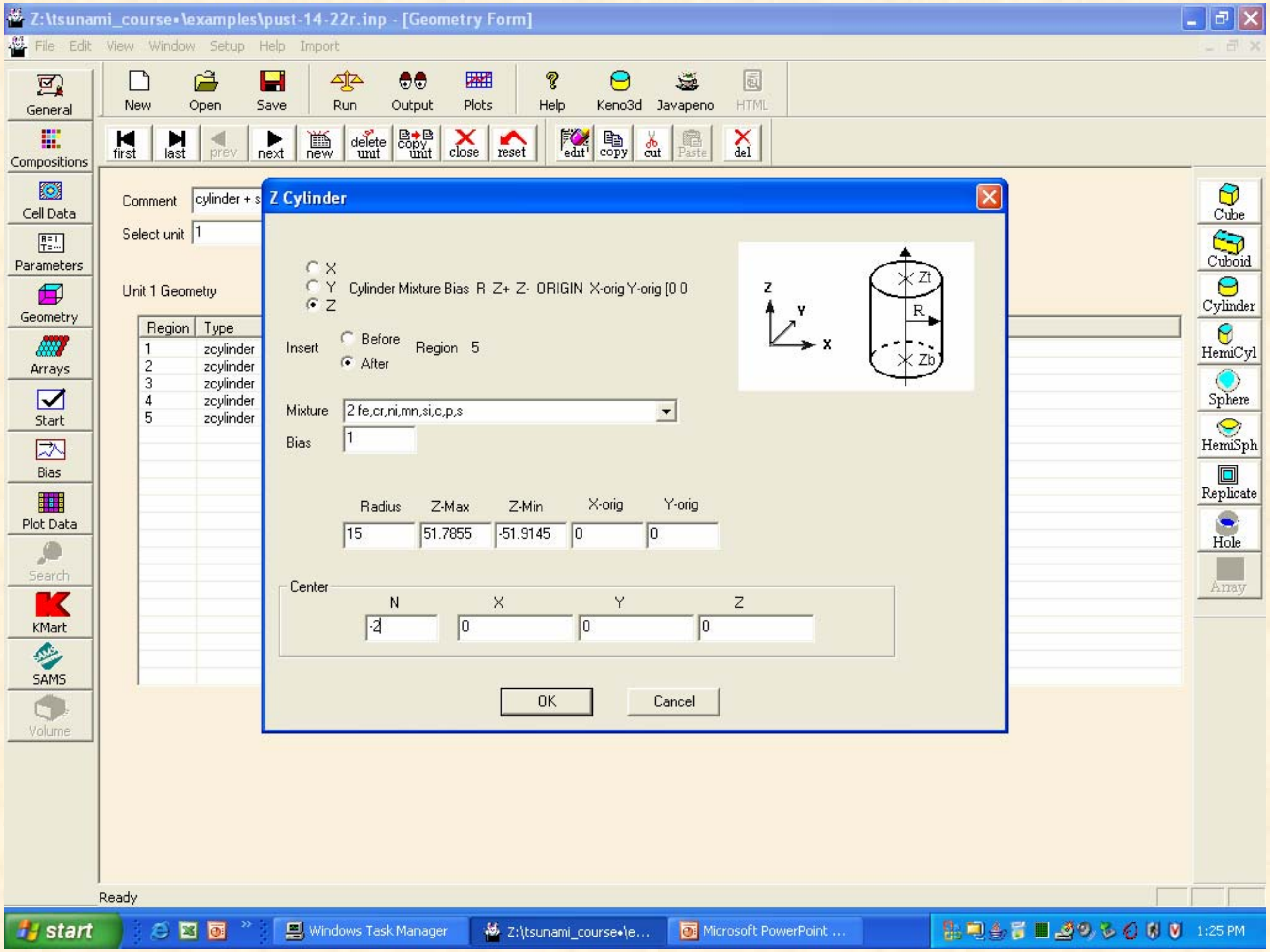
U(2)F_4 "Green Blocks" critical experiment
H/X = 294

Nuclide	Reaction	Direct Perturbation Sensitivity	TSUNAMI Sensitivity	% Diff.	TSUNAMI Sensitivity (no implicit)	% Diff.
^{1}H	total	0.22	0.22	0%	0.29	27%
^{19}F	total	0.04	0.04	0%	0.05	18%
^{235}U	total	0.25	0.25	0%	0.25	0%
^{238}U	total	-0.21	-0.21	0%	–0.29	39%

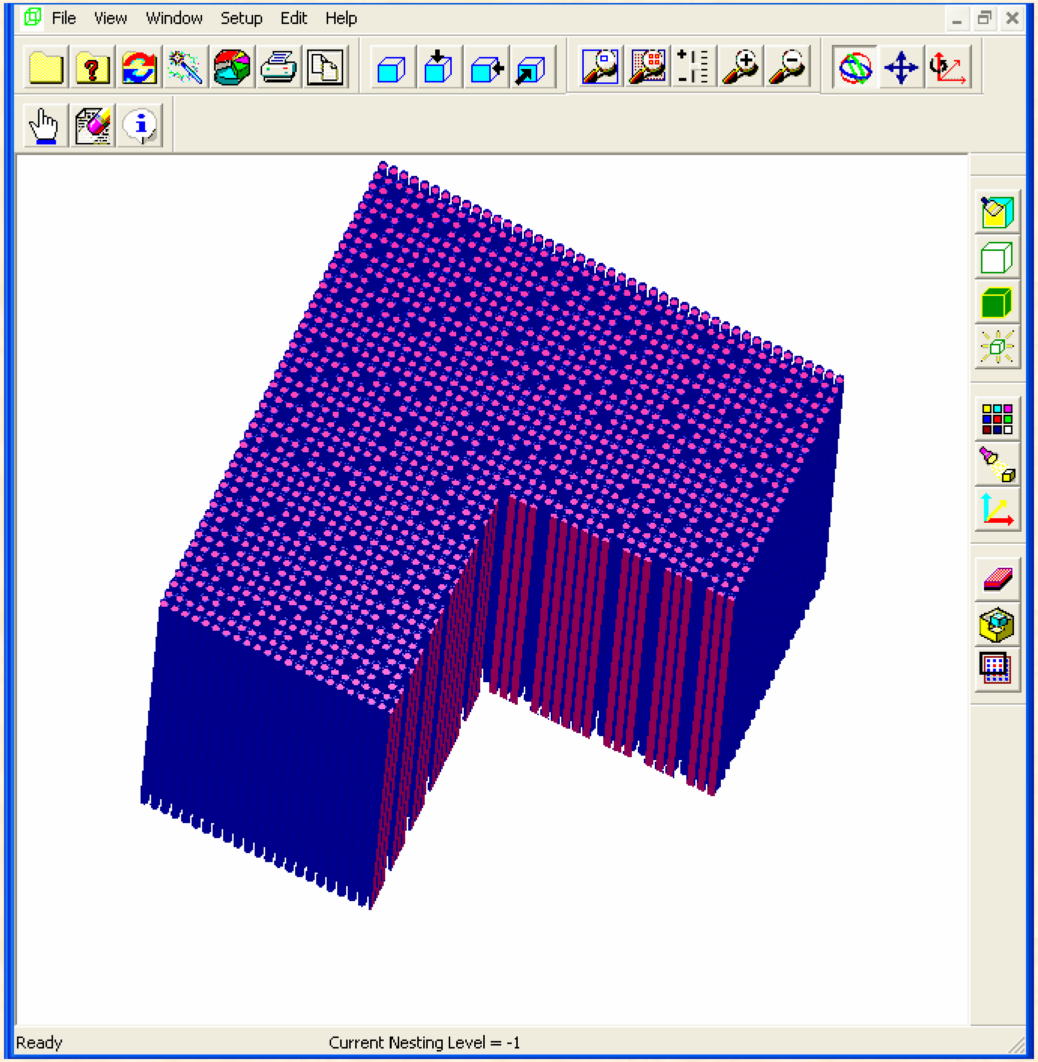
Sensitivity for ^{1}H Elastic, with Implicit Effect



GeeWiz Input GUI - TSUNAMI-3D



KENO3D Model Visualization



HTML Output

General Information

Input Data

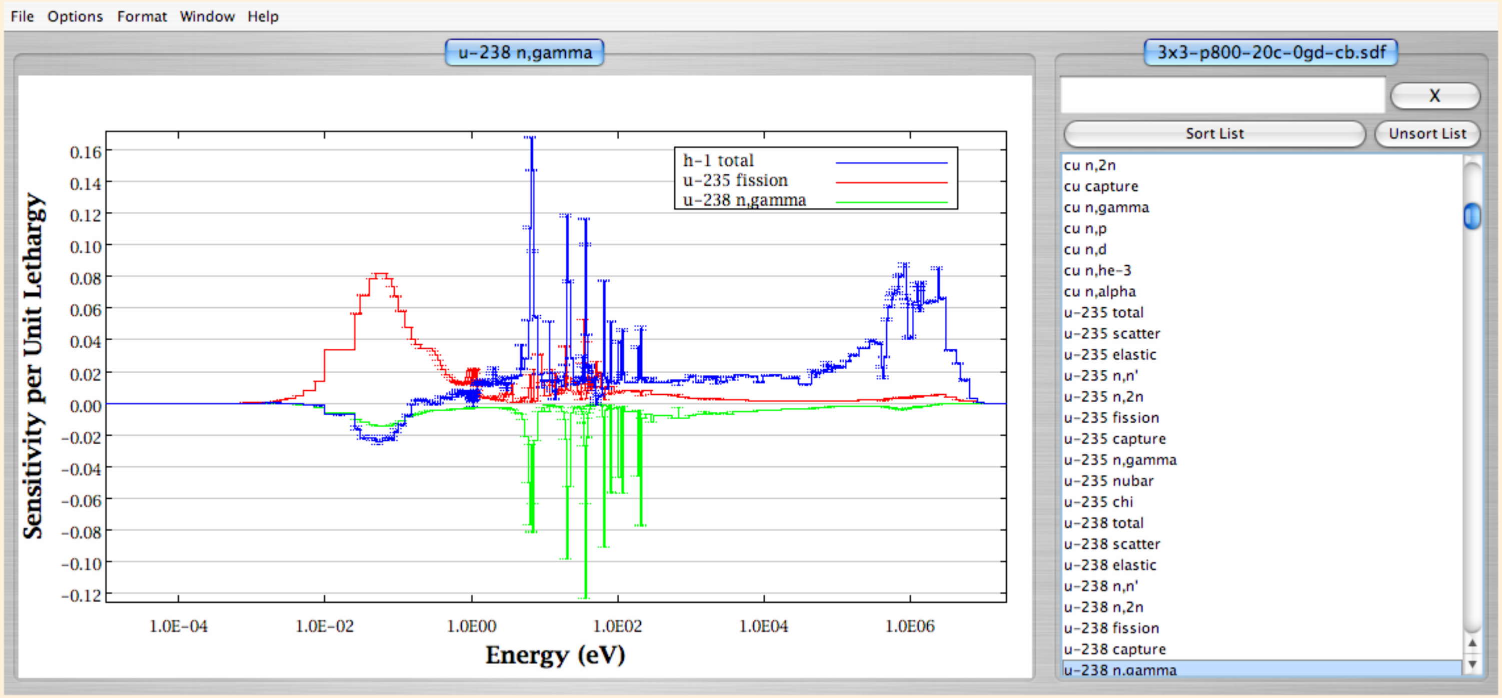
Results

- Energy, Region and Mixture Integrated Sensitivity Coefficients for this Problem
- Energy and Region Integrated Sensitivity Coefficients for this Problem
- Sensitivity Coefficients by Region
- Total Sensitivity Coefficients by Nuclide
- Total Sensitivity Coefficients by Mixture
- Sensitivity Data Plot
- Problem Characterization
- Uncertainty Information

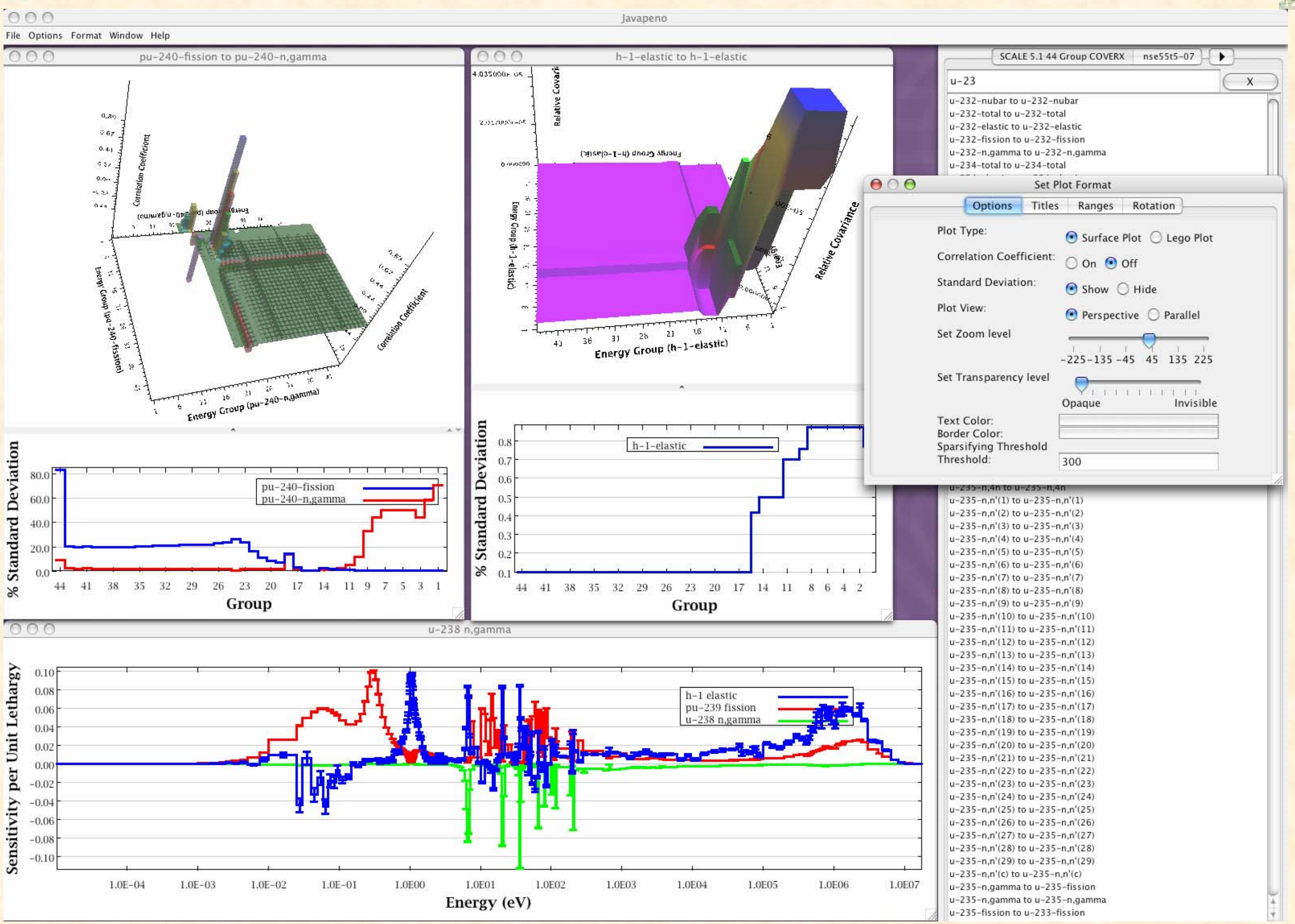
SAMS - Sensitivity Data Plot
u(2)f4 h/x=294

Plot of Sensitivity Data

Double-click an item on right side of window to plot, or select multiple items and right click to plot.

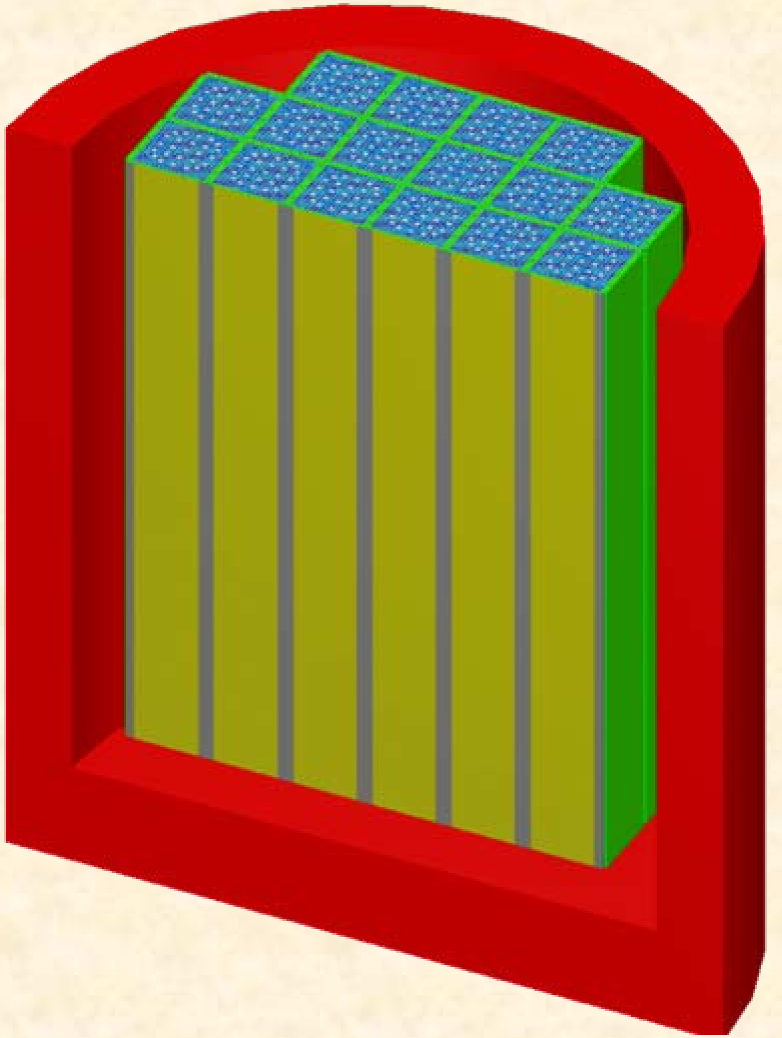


Javapeño for SCALE 5.1



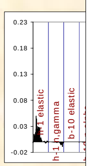
Applications of TSUNAMI-3D to Complex Models

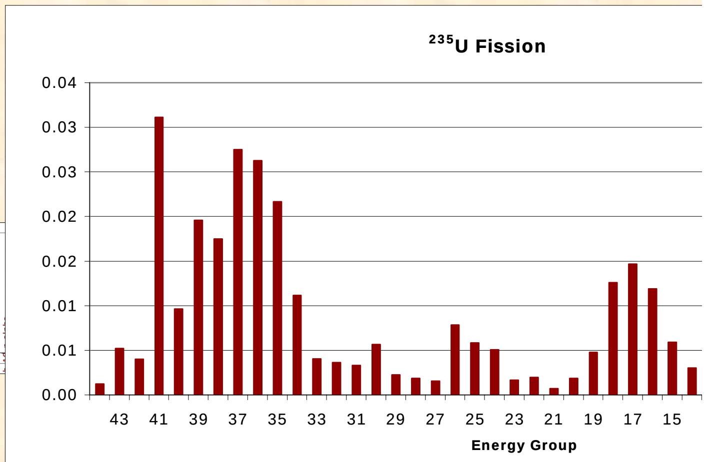
- Burnup Credit Cask Model
  - 32 PWR fuel assemblies in flooded cask
  - 18 axial burnup zones
  - Burned to 40 GWd/MTU; Cooled for 5 years
  - BORAL™ plates around each assembly
  - Cask filled with water
- Commercial Reactor Criticals (CRC)
  - Startup data from PWRs (Crystal River)
  - 1/2 core models
  - Each pin explicitly modeled with 18 axial zones
  - Sensitivity coefficients for ~47,000 nuclides, ~420,000 44-group profiles

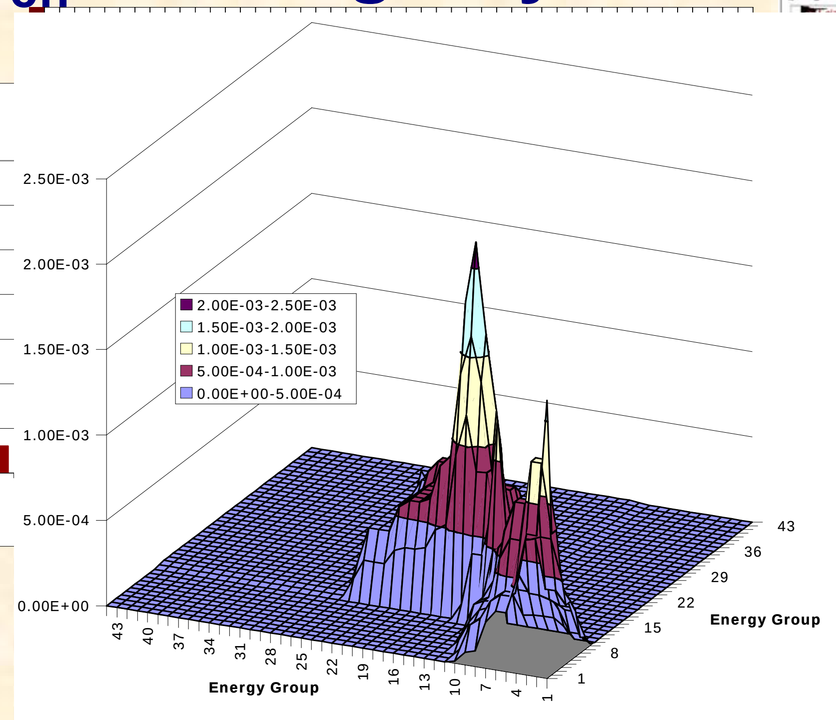


Uncertainty Propagation

- **Uncertainty in k_{eff} of a single system**







$$\frac{\Sigma}{k}\frac{dk}{d\Sigma}$$

$$= \sigma^2$$

C_{kk}

$$\left(\frac{\Delta k}{k}\right)^2$$

S^T

$$\frac{\Sigma}{k}\frac{dk}{d\Sigma}$$

$C_{\alpha\alpha}$

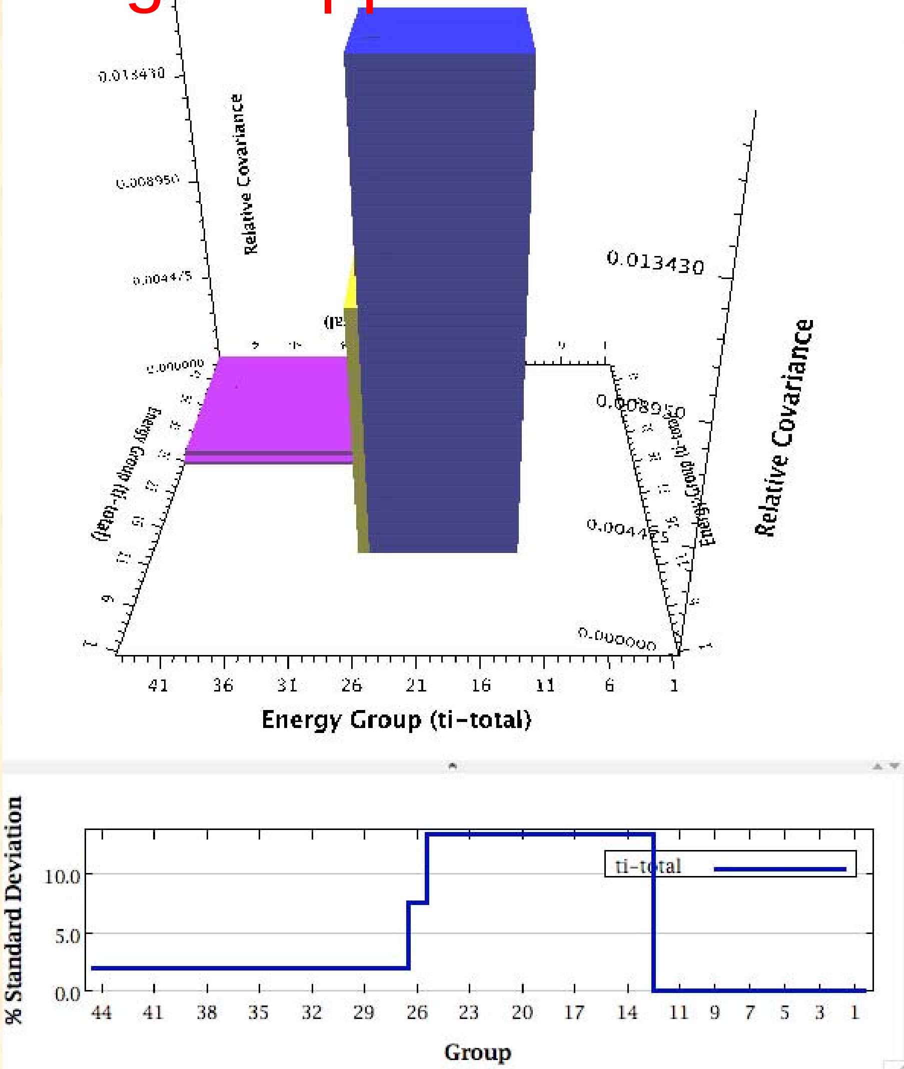
$$\left(\frac{\Delta\Sigma}{\Sigma}\right)^2$$

Procedure to Generate Covariance Library for Applications

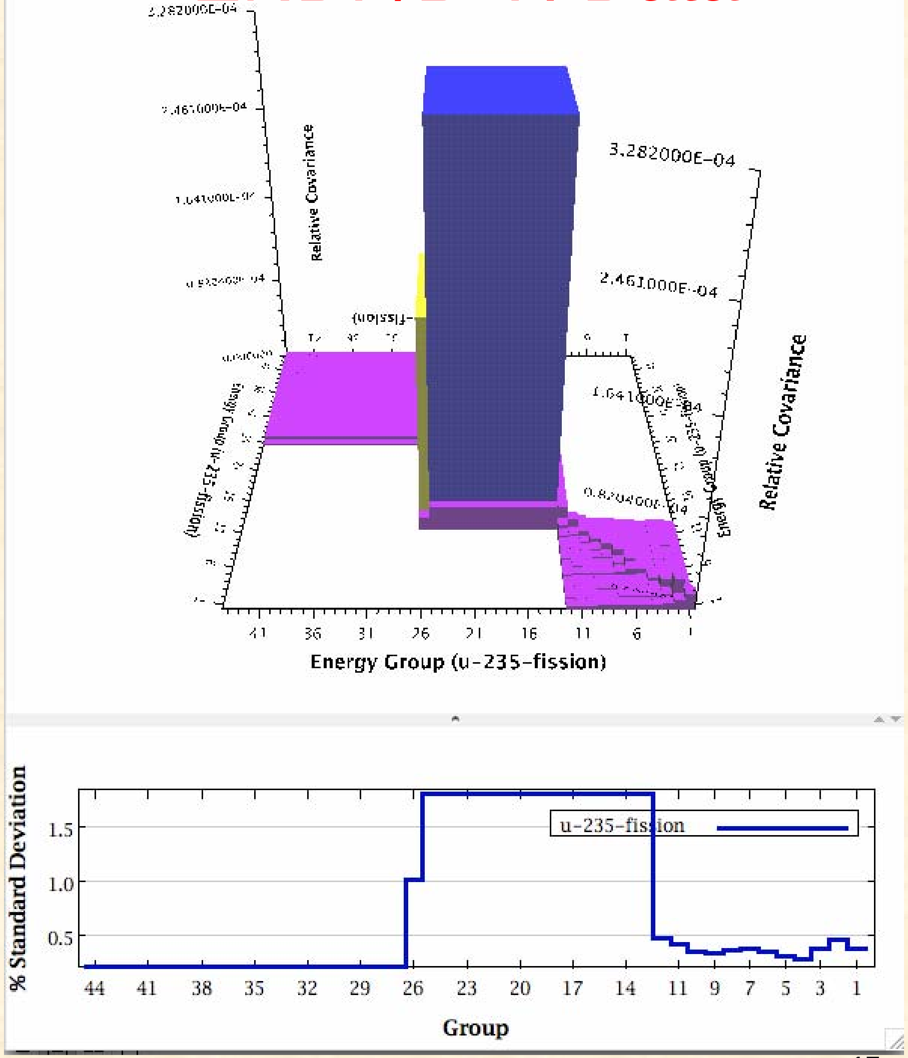
- Process all ENDF/B-VI covariances *(49 nuclides)*
- *ENDF/B-V covariances for 1 nuclide (^{10}B)*
- *JENDL 3.3 covariances for 7 nuclides*
- *CENDL 2 covariance for 2 nuclides*
- *JEF 3.1 covariances for 1 nuclide*
- *Fission spectrum, χ, data generated for 9 nuclides*
- Approximate covariances of other missing nuclides by **integral measurement uncertainties -** Mughabghab data *(>250 nuclides)*
  - **σ_c, σ_f, υ covariance for E<0.5 eV based thermal data uncertainty, with full correlation**
  - **σ_c, σ_f covariance for 0.5<E<5E3 eV based on resonance integral, with full correlation**
  - **σ_s covariance for moderators based on uncertainty in potential cross section, fully correlated**

Sample SCALE 5.1 Covariance Data

Integral Approximation Data



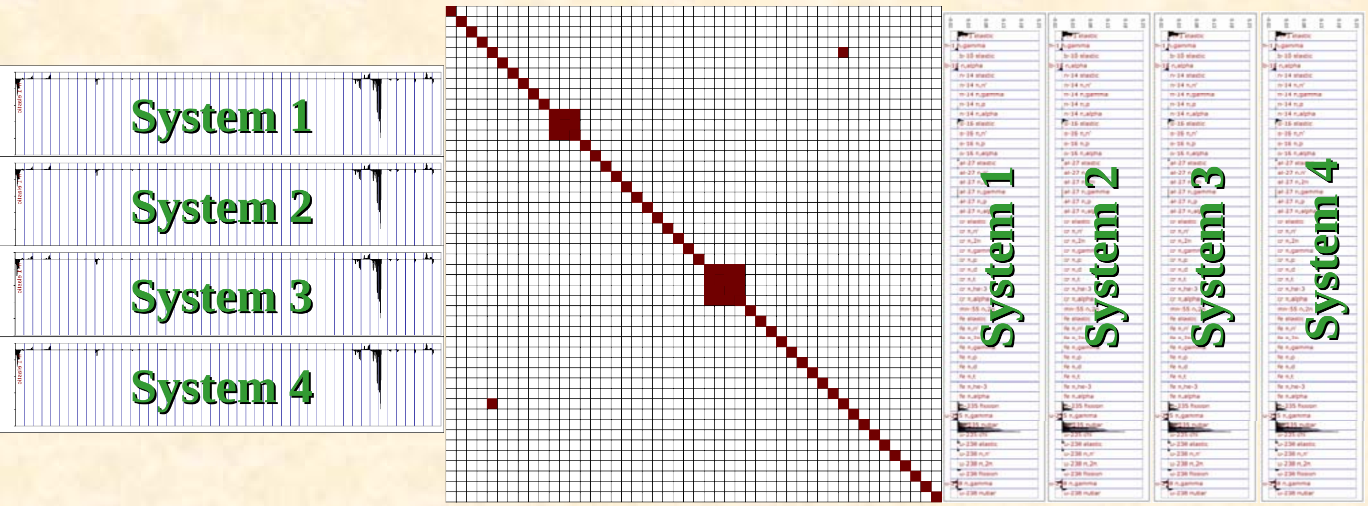
ENDF/B-VI Data



Uncertainty Propagation (con't)

- Uncertainty in k_{eff} for multiple systems

Diagonal elements are variance in each system



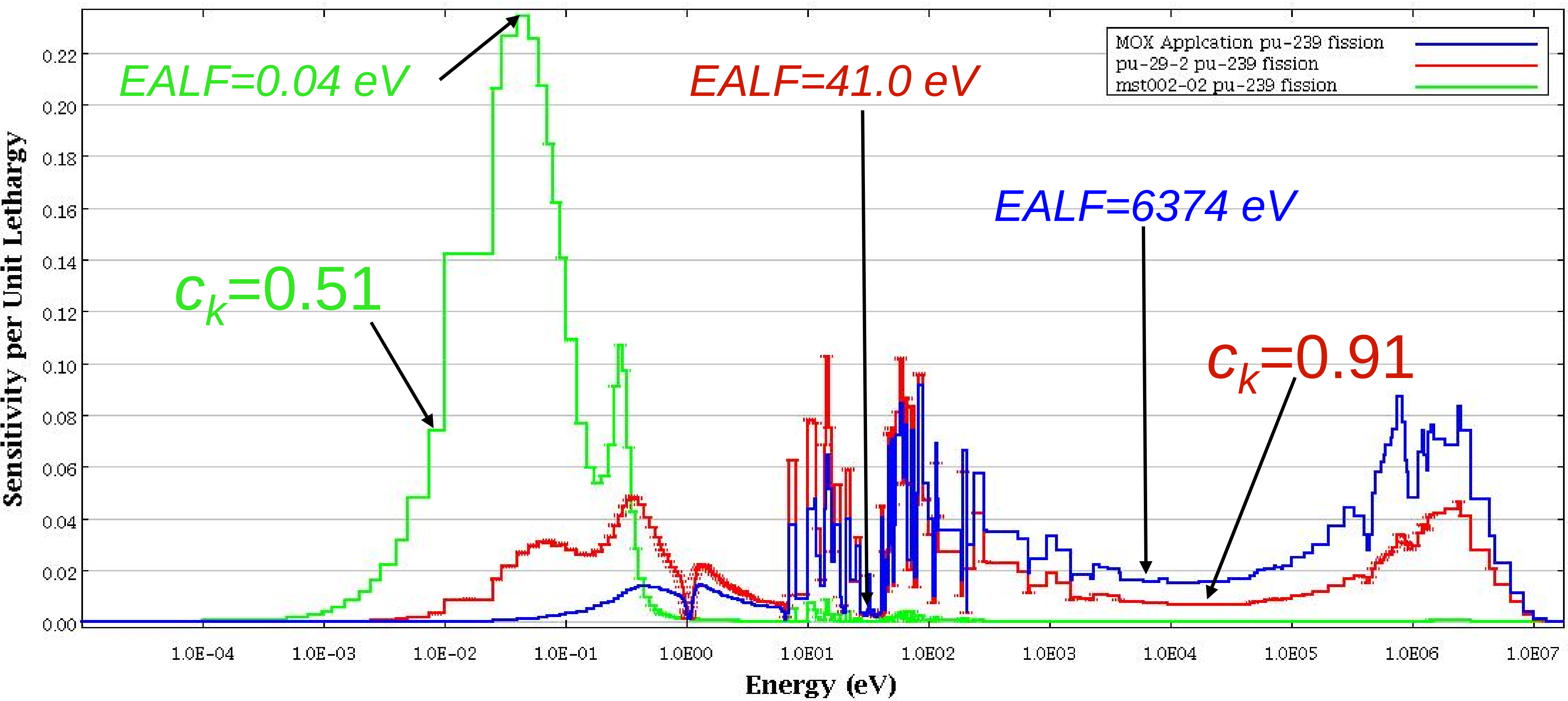
$$= \begin{bmatrix} \sigma_{11}^2 & \sigma_{12}^2 & \sigma_{13}^2 & \sigma_{14}^2 \\ \sigma_{21}^2 & \sigma_{22}^2 & \sigma_{23}^2 & \sigma_{24}^2 \\ \sigma_{31}^2 & \sigma_{32}^2 & \sigma_{33}^2 & \sigma_{34}^2 \\ \sigma_{41}^2 & \sigma_{42}^2 & \sigma_{43}^2 & \sigma_{44}^2 \end{bmatrix}$$

Off-diagonal elements are covariance between two systems

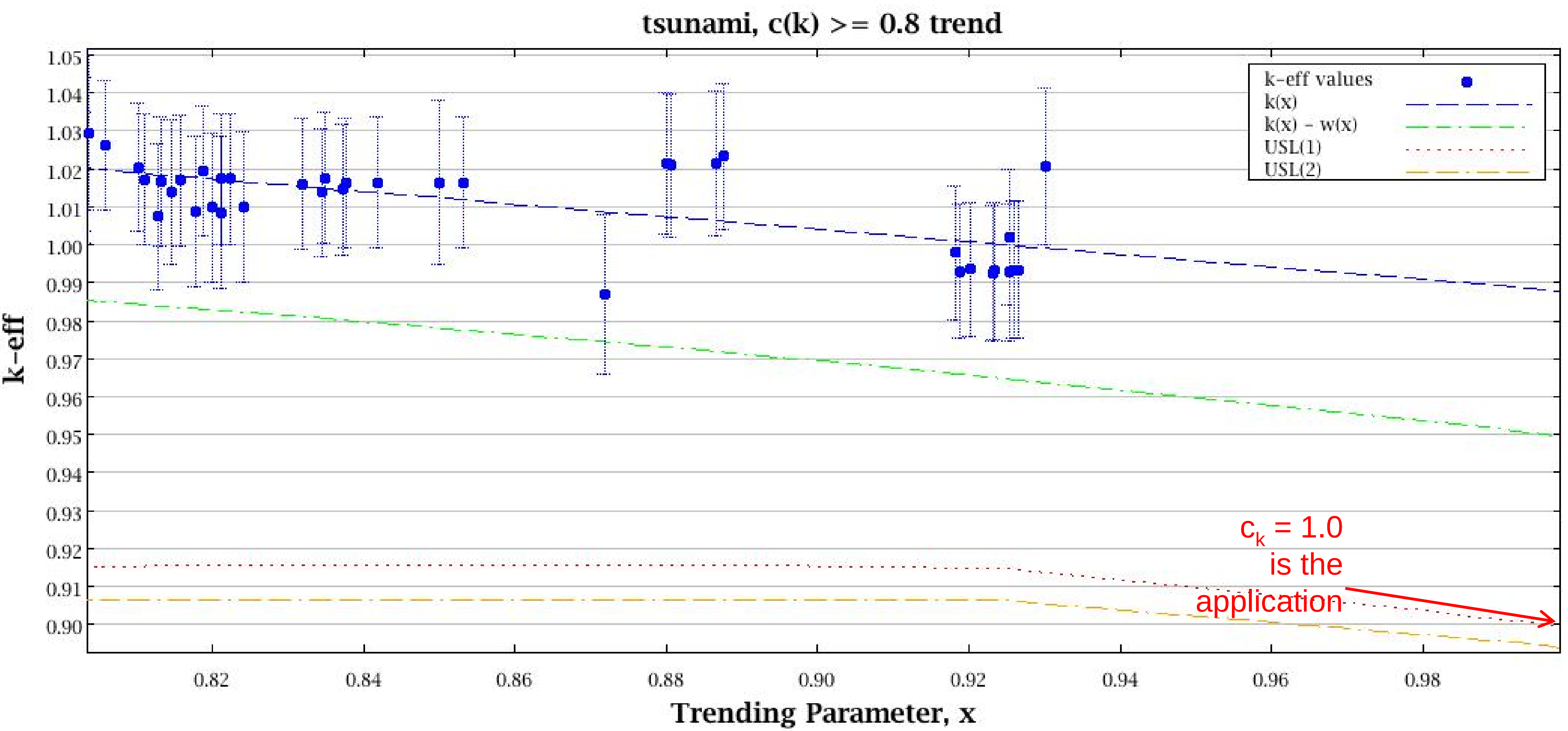
- Correlation coefficient between two systems:

$$c_k = \frac{\sigma_{21}^2}{\sqrt{\sigma_{11}^2}\sqrt{\sigma_{22}^2}}$$

^{239}Pu Fission Sensitivity

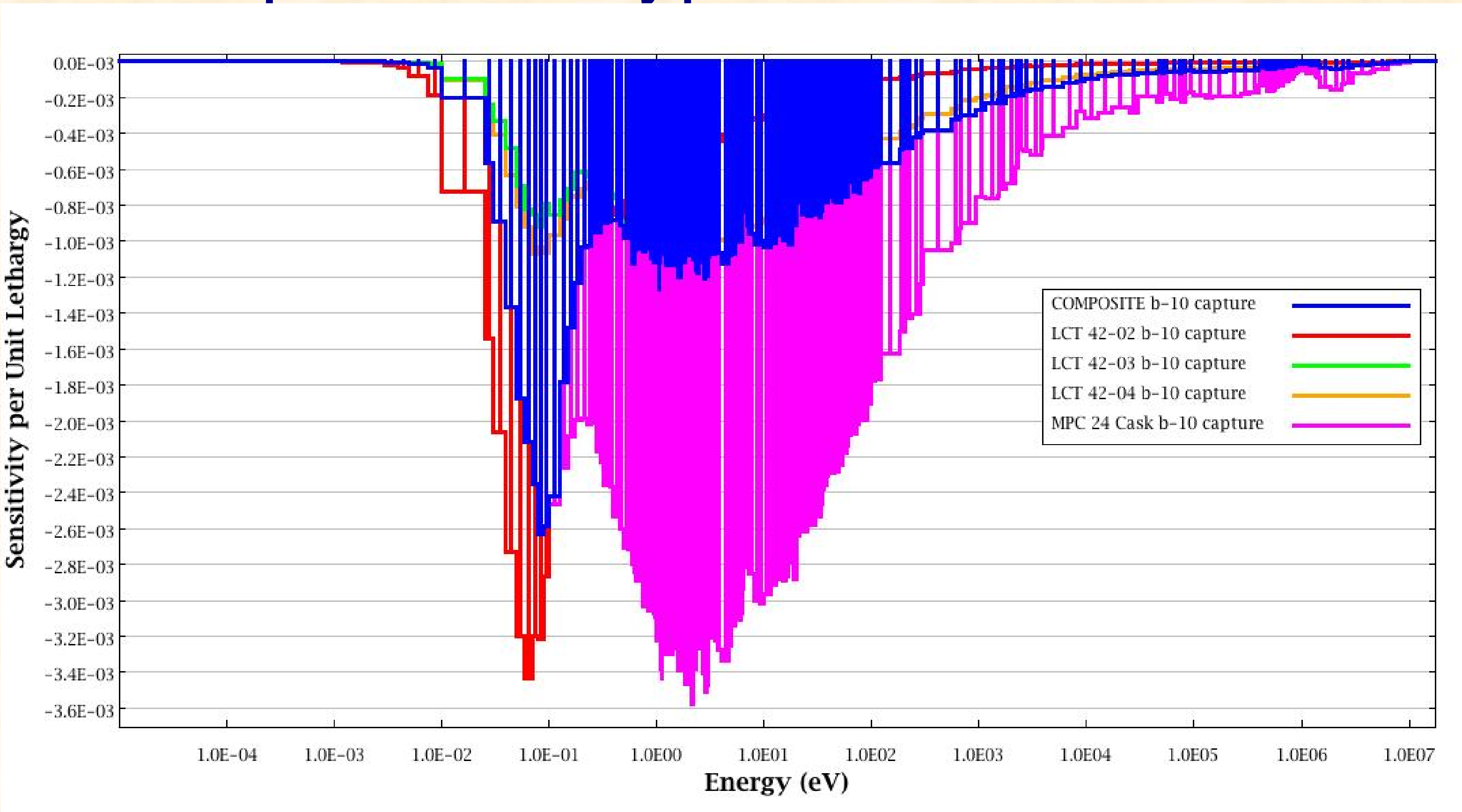


Trend with $c_k \geq 0.8$ USL = 0.90



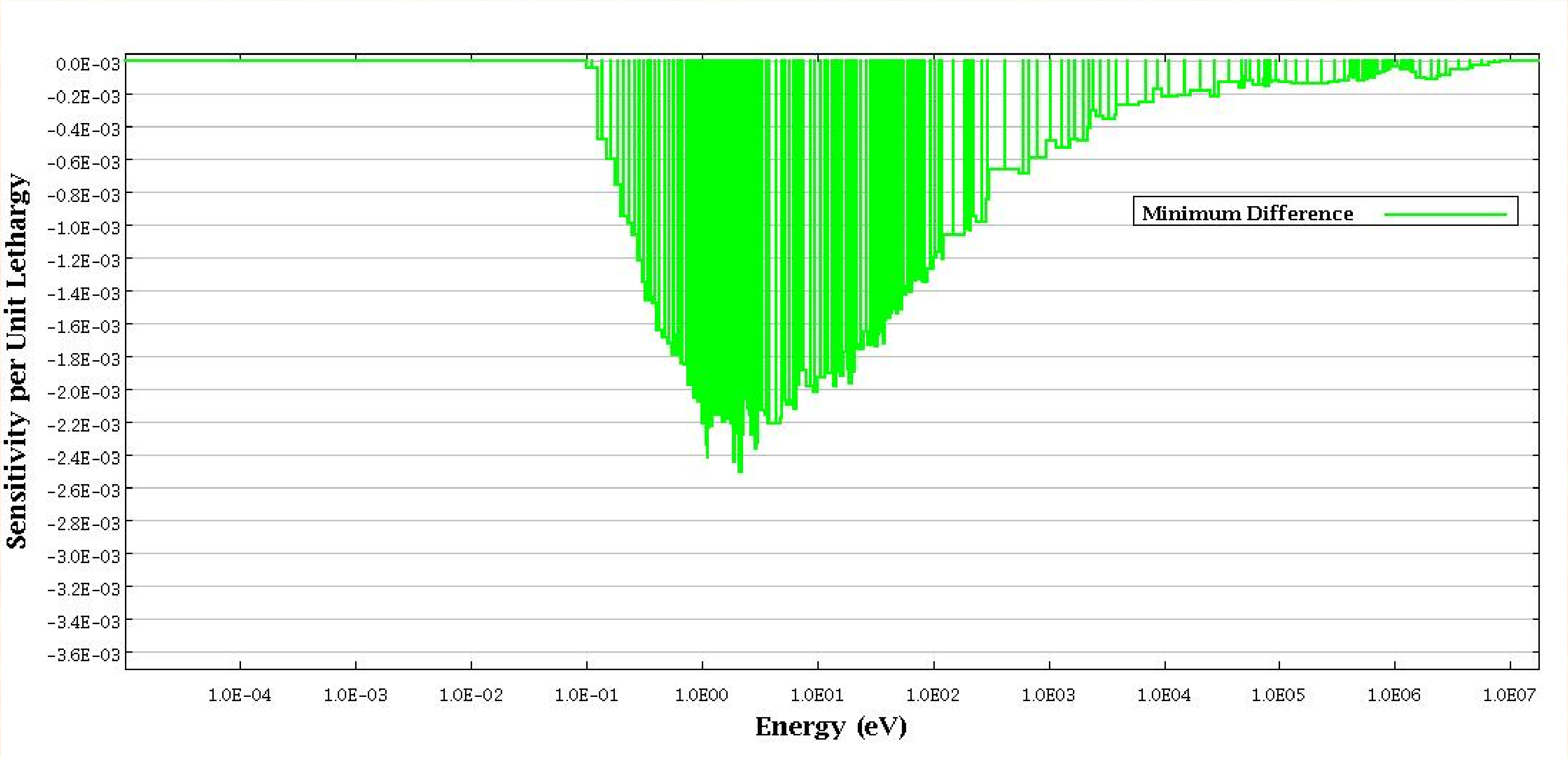
Composite Sensitivity Data

- **Coverage produced by several experiments can be "built up" as a composite sensitivity profile.**



Minimum Differences

- Difference between sensitivity profiles for the application and the composite show portion of application data that is not covered by experiments.



Penalty Assessment

- Penalty is an additional margin to subcriticality due uncertainty in cross sections that are not covered by benchmarks
- Penalty can be assessed by propagating uncovered sensitivity data to k_{eff} through cross-section-covariance data.
- Calculation is similar k_{eff} uncertainty due to cross sections, but minimum differences (Z_a) replace application sensitivities.

$$\Delta k_{eff} / k_{eff} = \sqrt{\mathbf{Z_a} \mathbf{C}_{\alpha\alpha} \mathbf{Z_a}^{\dagger}}$$

Reduced uncertainties

Application Uncertainty
0.77%

Covariance Matrix		% Δk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{235}U nubar	^{235}U nubar	6.3800E-01 ± 2.2348E-05
^{235}U n,gamma	^{235}U n,gamma	3.0069E-01 ± 2.0102E-05
^{238}U n,gamma	^{238}U n,gamma	2.3836E-01 ± 1.7811E-05
^{235}U fission	^{235}U fission	1.6262E-01 ± 1.3586E-05
^{1}H elastic	^{1}H elastic	7.0789E-02 ± 6.6674E-04
^{1}H n,gamma	^{1}H n,gamma	6.7436E-02 ± 4.2071E-06
Zr n,gamma	Zr n,gamma	5.7816E-02 ± 9.1843E-06
^{238}U fission	^{238}U fission	4.3381E-02 ± 5.0644E-06

Penalty Uncertainty
(due to uncovered sensitivities)
0.20%

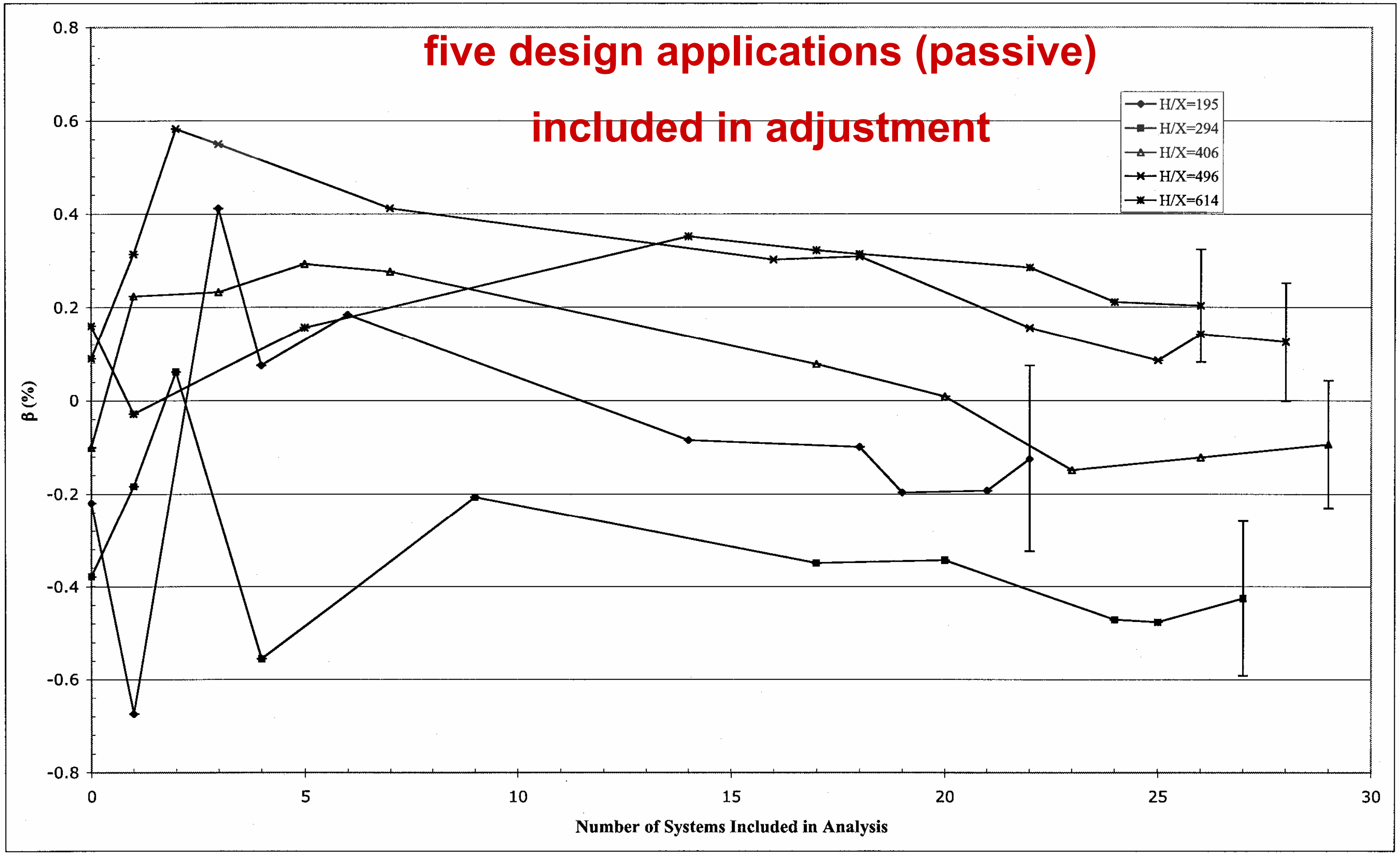
Covariance Matrix		% Δk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{235}U chi	^{235}U chi	1.7757E-01 ± 2.2553E-05
Zr n,gamma	Zr n,gamma	5.7816E-02 ± 9.1843E-06
^{235}U nubar	^{235}U nubar	5.6465E-02 ± 6.6658E-06
^{238}U n,n'	^{238}U n,n'	2.8220E-02 ± 1.6134E-04
^{1}H n,gamma	^{1}H n,gamma	2.7224E-02 ± 4.3928E-06
^{235}U fission	^{235}U fission	1.7398E-02 ± 6.9908E-06
^{16}O n,alpha	^{16}O n,alpha	1.2838E-02 ± 1.2354E-05
^{1}H elastic	^{1}H elastic	8.3229E-03 ± 2.0752E-03

TSURFER

Performs *Generalized Linear Least-Squares (GLLS)* Analysis of Design System and Benchmark Data Base

- **Systematic procedure to consolidate calculations with measured responses**
- **Computes “best” cross-section adjustments to minimize differences in computed and measured benchmark responses**
- **Propagation of data perturbations to the design system response provides estimate of computational bias and uncertainty**
- **Allows correlations in experimental uncertainty components; filtering of benchmarks based on similarity; edit of adjusted data and covariances**

Bias Prediction Versus Number of Similar Systems ($c_k > 0.9$) in GLLS Adjustment



Reactivity Sensitivity and Uncertainty Analysis

$$S_{\rho,\alpha} = \frac{\alpha \partial \rho_{1\to 2}}{\rho_{1\to 2} \partial \alpha}$$

Eigenvalue Differencing Approach

$$S_{\rho,\alpha} = \left\{ \frac{\left\langle \Phi_1^* \left(\frac{\alpha \partial L_1}{\partial \alpha} - \lambda_1 \frac{\alpha \partial P_1}{\partial \alpha} \right) \Phi_1 \right\rangle}{\rho_{1\to 2} \left\langle \Phi_1^* P_1 \Phi_1 \right\rangle} - \frac{\left\langle \Phi_2^* \left(\frac{\alpha \partial L_2}{\partial \alpha} - \lambda_2 \frac{\alpha \partial P_2}{\partial \alpha} \right) \Phi_2 \right\rangle}{\rho_{1\to 2} \left\langle \Phi_2^* P_2 \Phi_2 \right\rangle} \right\}$$

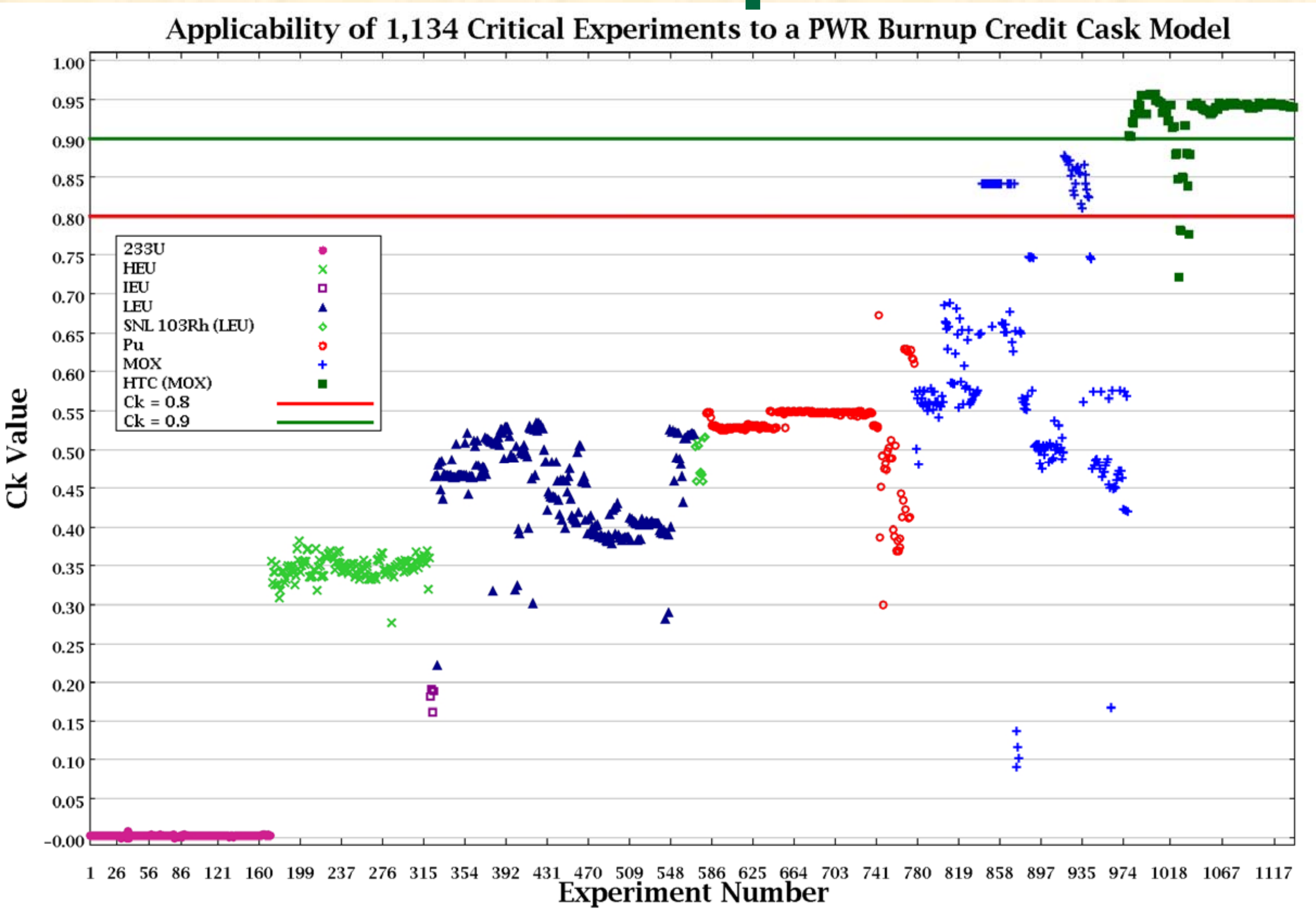
Uncertainty in Reactivity

$$\sigma_\rho^2 = \left(\frac{\lambda_1 \sigma_{\lambda_1}}{\rho_{1\to 2}} \right)^2 + \left(\frac{\lambda_2 \sigma_{\lambda_2}}{\rho_{1\to 2}} \right)^2 - 2 \frac{\sigma_{\lambda_1,\lambda_2}}{\sigma_{\lambda_1} \sigma_{\lambda 2}} \left(\frac{\lambda_1 \sigma_{\lambda_1}}{\rho_{1\to 2}} \right) \left(\frac{\lambda_2 \sigma_{\lambda_2}}{\rho_{1\to 2}} \right)$$

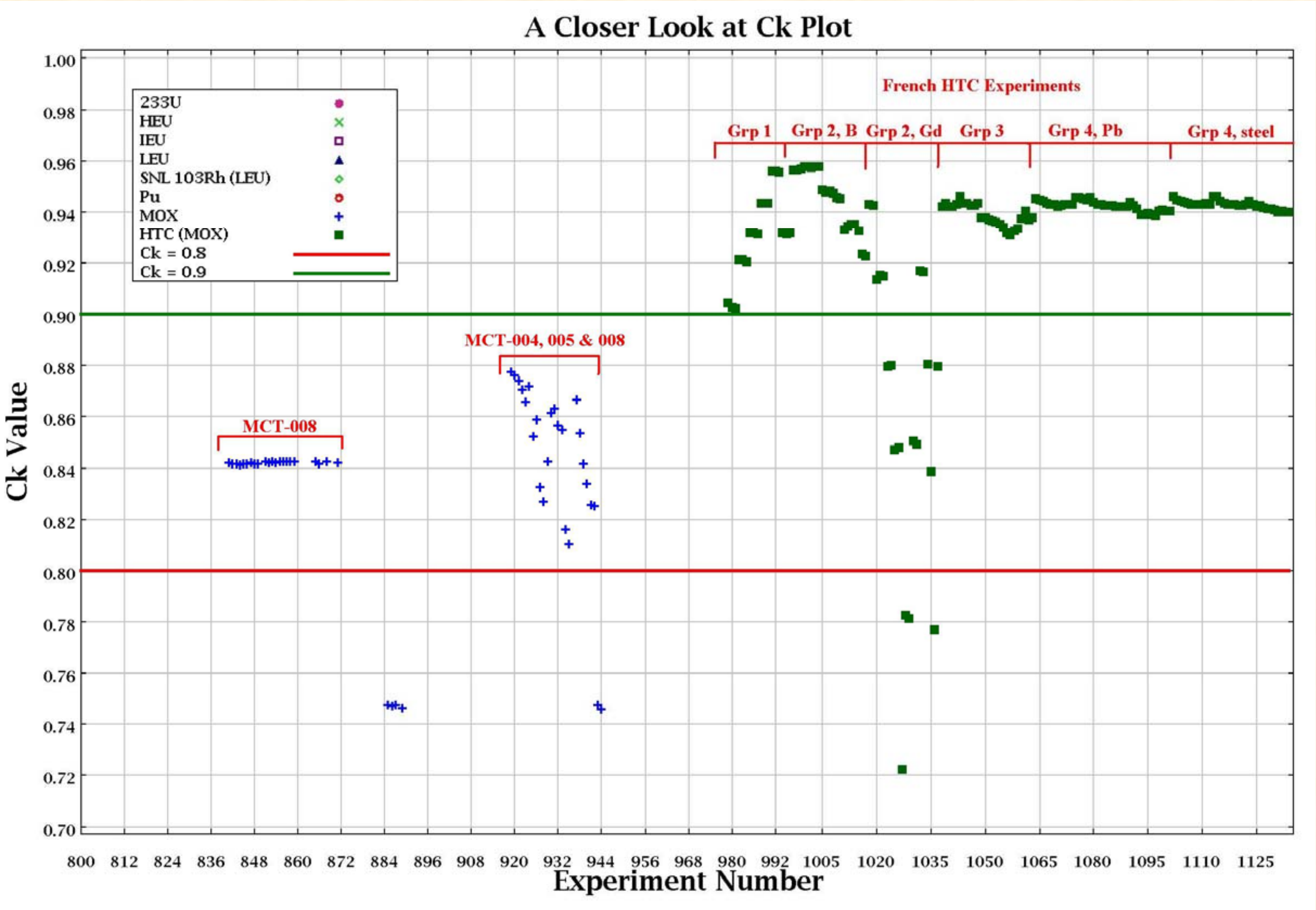
Practical Uses of TSUNAMI

- Validation/Experiment Applicability Studies
  - Yucca mountain, Burnup credit, MOX fresh fuel, MOX fuel fabrication facility, Poisoned basket studies
- Experiment Design Optimization
  - >5 wt-% fuel
    - NERI with Areva, Sandia National Laboratories, and University of Florida
    - 7% Experiments to be assembled at SNL January 2007
  - Additional >5% experiment design work for Toshiba
  - Space Nuclear Power - General Physics Experiments
- Atomic Energy of Canada, Limited - ACR-1000 Code Validation

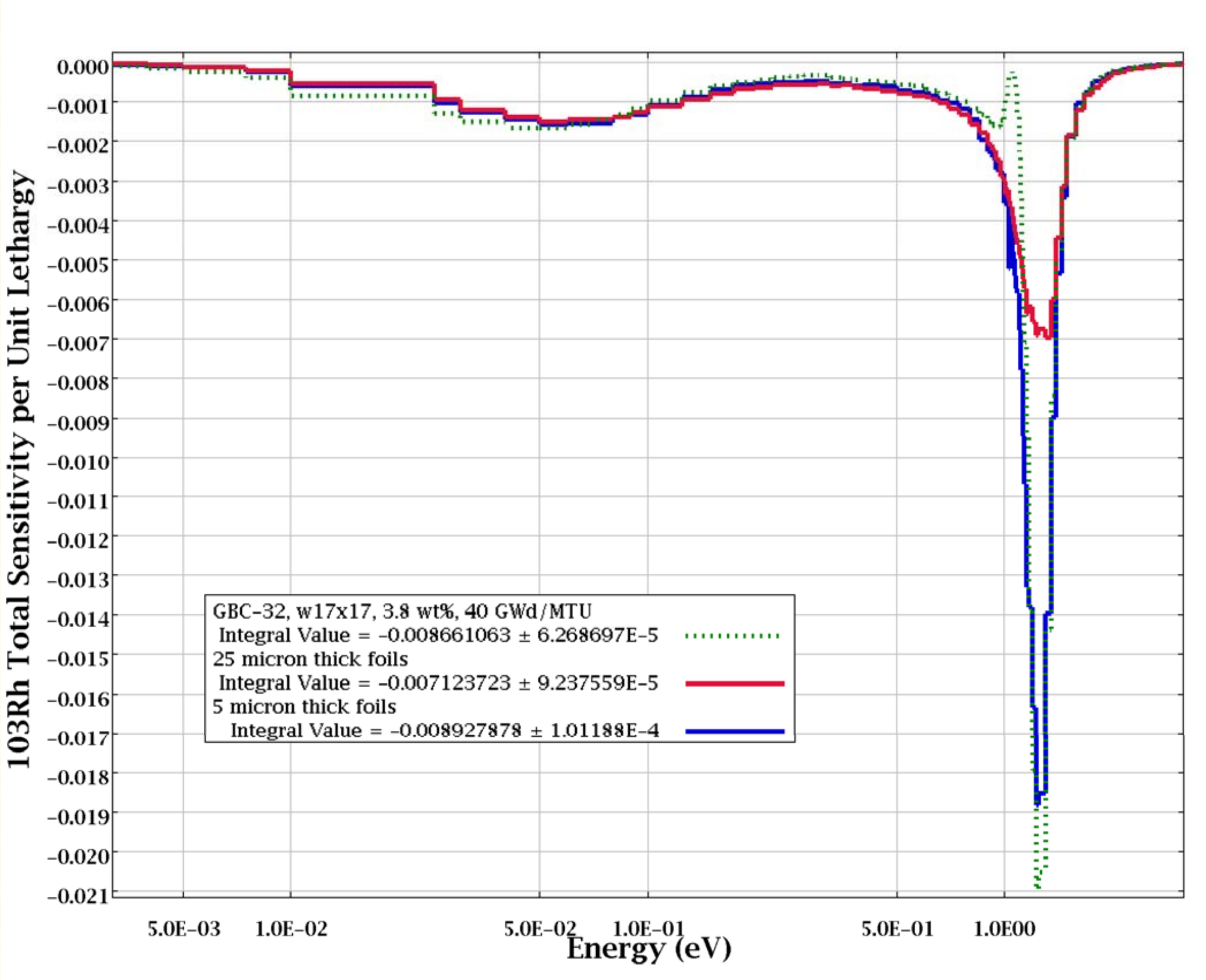
Burnup Credit: c_k for GBC-32 with >1100 Critical Experiments



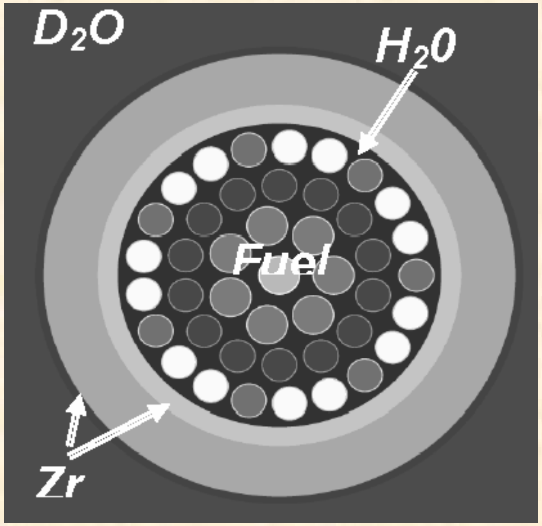
Burnup Credit: c_k for GBC-32 with >1100 Critical Experiments

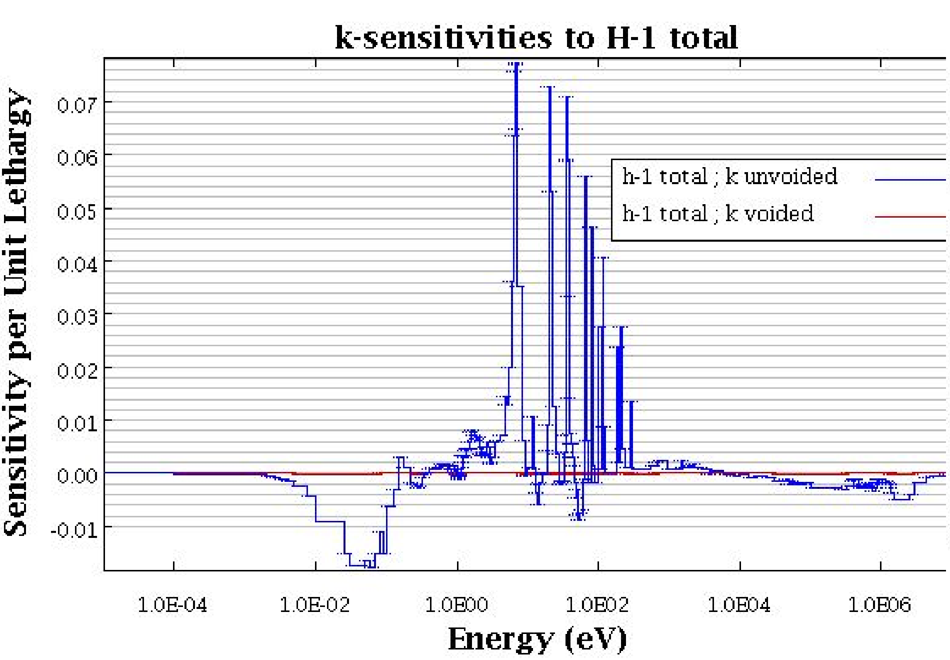


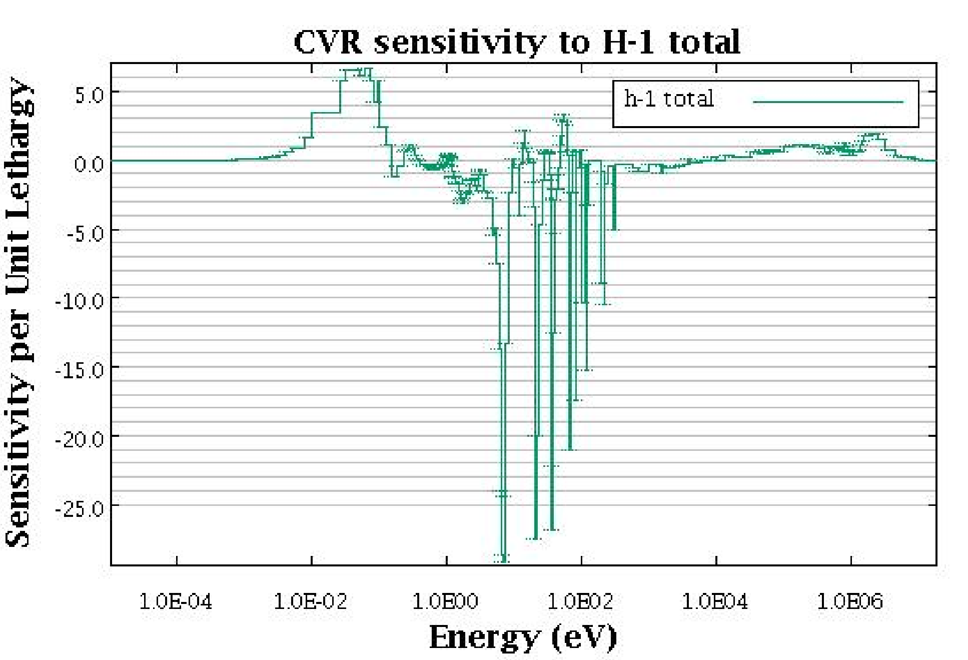
Burnup Credit: Rh-103 Sensitivity from SNL BUCCX and GBC-32 Cask



Application to ACR-700 CVR







ACR-700 Uncertainties

TABLE V
Response Uncertainties Due to Available Nuclear Data Covariances

Response	Relative Standard Deviation (%)
Multiplication factor for state 1	0.80
Multiplication factor for state 2	0.84
Coolant void reactivity (CVR)	49.8

ORNL Production-Level S/U Capabilities

- **Publicly released TSUNAMI tools in SCALE 5.0**
- **Specifically mentioned in NRC's ISG-10 for criticality code validation**
- **TSUNAMI training for criticality code validation**
  - **8 multiday classes taught since 2004, ~150 participants**
  - **6-hour tutorial presented at 2004 ANS annual meeting**
  - **Next training course in November 2006**

Possible additions to TSUNAMI

- 2D Deterministic Eigenvalue Capability
- Revitalization of ORNL Generalized Perturbation Theory Capabilities for Reactor Physics Responses
  - 1D, 2D, 3D deterministic (refreshed)
  - 3D Monte Carlo (new R&D required)
- Resonance self-shielding implicit effect for cell homogenization and double-heterogeneity calculations
- 2D continuous energy deterministic code for resonance self shielding
- Perturbation theory for continuous energy Monte Carlo calculations
- Porting codes to large-scale computers